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Progress towards an effective model for FeSe from high-accuracy first-principles quantum Monte Carlo[1] BRIAN BUSEMEYER, LUCAS K. WAGNER, Univ of Illinois - Urbana — While the origin of superconductivity in the iron-based materials is still controversial, the proximity of the superconductivity to magnetic order is suggestive that magnetism may be important. Our previous work has suggested that first-principles Diffusion Monte Carlo (FN-DMC) can capture magnetic properties of iron-based superconductors that density functional theory (DFT) misses, but which are consistent with experiment. We report on the progress of efforts to find simple effective models consistent with the FN-DMC description of the low-lying Hilbert space of the iron-based superconductor, FeSe. We utilize a procedure outlined by Changlani et al.[1], which both produces parameter values and indications of whether the model is a good description of the first-principles Hamiltonian. Using this procedure, we evaluate several models of the magnetic part of the Hilbert space found in the literature, as well as the Hubbard model, and a spin-fermion model. We discuss which interaction parameters are important for this material, and how the material-specific properties give rise to these interactions.

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